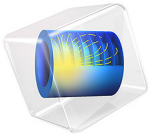


Transport Phenomena in a Polymer Electrolyte Fuel Cell Membrane-Electrode Assembly

Introduction

The membrane-electrode assembly (MEA) of a polymer electrolyte membrane fuel cell is the core component of the fuel cell system. The central part of the MEA is the polymer electrolyte membrane, which acts as a gas separator and ion conductor. Porous catalytic layers (gas diffusion electrodes) are located adjacent to the membrane, one on each side. The catalytic layers contain three separate phases: gas pores for the reactants, an electron-conducting electrode phase and an ion-conducting polymer (ionomer) electrolyte phase. The surface of the electrode phase in the catalytic layers contain noble metal catalysts in order to minimize the reaction overpotentials. Gas diffusion layers (GDLs) are placed outside the catalytic layers. The GDLs are also porous and perform the task of conducting electrons and allowing the passage of gases.

For low-temperature fuel cells, water management is of crucial importance for the performance of the MEA. Running the cell under too wet conditions may result in mass transport limitations of gases due to flooding of liquid water in the pores, whereas running the cell under too dry conditions may result in poor performance due to a low ohmic conductivity in the ionomer used in the membrane and catalytic layers.

This tutorial models how the relative humidity of the inlet gases impacts the performance of a low-temperature polymer electrolyte MEA. The model includes gas phase mass transport, water transport in the ionomer and humidity-dependent ionomer conductivity. The model non-isothermal, with the electrochemical reactions and Joule heating in the electrodes and ionomer giving rise to heat sources. Hydrogen cross-diffusion over the ionomer membrane is also included in the model.

Model Definition

GEOMETRY

The model is defined in 1D and includes the anode and cathode GDLs, catalytic layers and the ionomer membrane. The GDLs are further divided into a two separate layers, one macroporous and one microporous layer (MPL), where the MPL is located toward the membrane. The model geometry is shown in Figure 1.

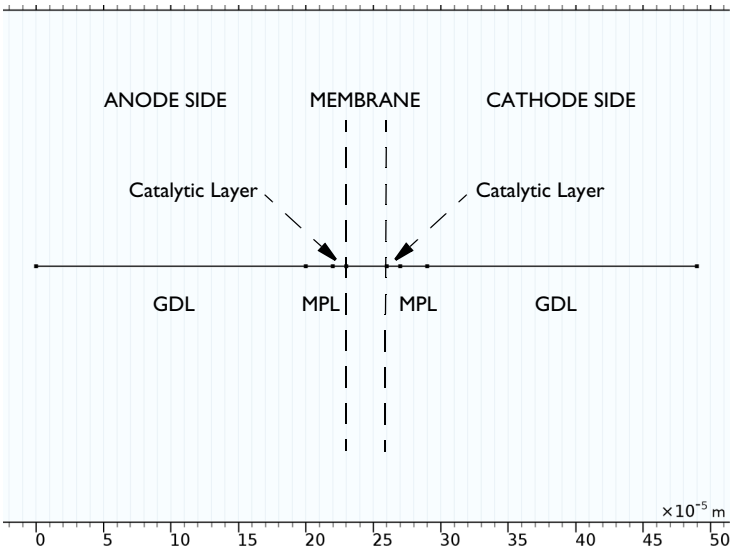


Figure 1: Model geometry.

The following two physics interfaces are used to describe the different coupled phenomena:

- Hydrogen Fuel Cell
- Heat Transfer

The Hydrogen Fuel Cell interface is used to describe the transfer of charge in the electrode and electrolyte (ionomer) phases using Ohm's law, where the ionomer conductivity depends on the water content as will be described below. Concentration-dependent kinetic expressions are used to set up the anodic and cathodic porous electrode charge transfer reactions. The Hydrogen Fuel Cell interface is also used to model the mass transfer of the species in the gas phases on each side of the membrane using the Maxwell-Stefan equations. The mass fractions of hydrogen and water vapor are solved for on the anode side. On the cathode side, the mass fractions of nitrogen, oxygen, and water vapor are solved for. Source terms related to the porous electrode reactions and water phase transfer are added in the catalytic layer domains.

The Membrane Transport features of the Hydrogen Fuel Cell interface are used to model the transport of water in the ionomer phase in the catalytic layer and the membrane domains. The molecular flux of water depends both on chemical potential gradient-driven

permeation and electroosmotic drag, using experimentally estimated parameters available in the Nafion material in the Fuel Cell and Electrolyzer Material Library.

WATER UPTAKE AND IONOMER PROPERTIES

To describe the water and charge transport in the ionomer, additional expressions and data for ionomer conductivity and water activity and diffusivity in the ionomer are required. The water activity will be used to define the water transfer rate between the gas and ionomer phases. The water uptake parameter λ (dimensionless) defines the water content of the ionomer as

$$\lambda = c\frac{M_{\mathrm{EW}}}{\rho_{\mathrm{ionomer}}} \tag{1}$$

where c (SI unit: mol/m^3) is the water concentration, M_{EW} (SI unit: kg/mol) the equivalent weight and ρ_{ionomer} (SI unit: kg/m^3) the ionomer density. The equivalent weight is defined as the molecular mass of the ionomer per sulfonic acid group attached to the polymer backbone.

The water activity in the ionomer phase, $a_{\mathrm{H_2O,\,ionomer}}$ (dimensionless), and λ are interrelated using an empirical expression the Nafion material node in the material library as, shown in Figure 2.

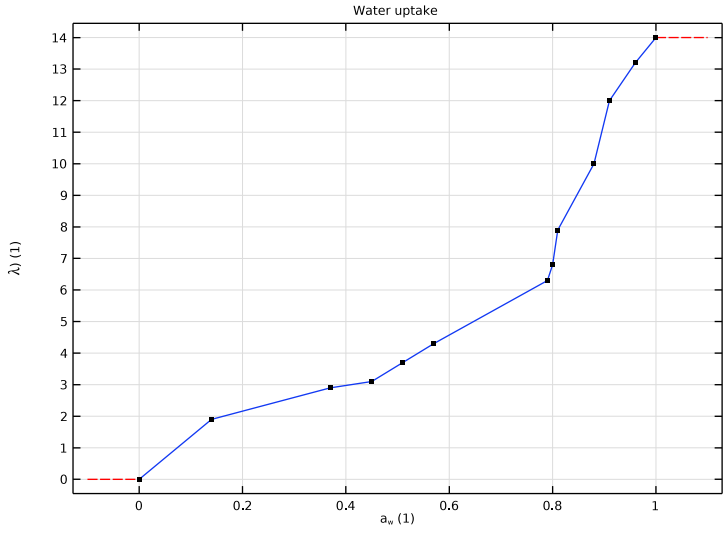


Figure 2: Water uptake versus water activity in the ionomer.

The electrolyte conductivity σ_l (SI unit: S/m) is defined as a function of both temperature and relative humidity as shown in Figure 2.

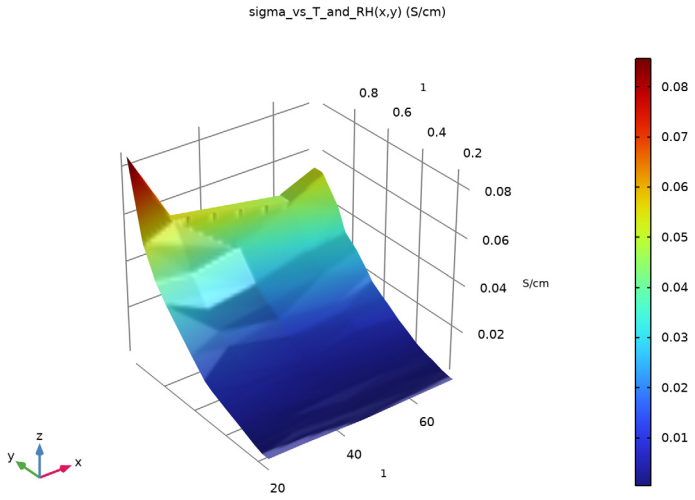


Figure 3: Electrolyte conductivity versus temperature and relative humidity.

HYDROGEN CROSS-OVER TRANSPORT THROUGH THE MEMBRANE

Hydrogen diffusing from the anode side through the membrane is assumed to be oxidized as soon as it reaches the cathode catalytic layer according to:

$$H_2(\text{mem}) \rightarrow 2H^+ + 2e^- \tag{2}$$

Assuming the hydrogen concentration to be zero at the membrane-cathode catalytic boundary and in equilibrium with gaseous hydrogen on the anode side, the flux of hydrogen though the membrane is defined as

$$J_{\text{H2,ionomer}} = \frac{\Psi_{\text{H2}} p_{\text{H2, gas, anode}}}{L_{\text{mem}}} \tag{3}$$

where Ψ_{H2} (SI unit: m^2/s) is the hydrogen permeation coefficient in the ionomer (incorporating the hydrogen gas-ionomer phase transfer partition constant) and L_{mem} is the membrane thickness.

The hydrogen oxidation current is added to the charge balance as a boundary electrolyte current density contribution

$$i_{\mathrm{H2}} = 2FJ_{\mathrm{H2,ionomer}} \tag{4}$$

WATER MEMBRANE-GAS PHASE TRANSFER

The water transfer rate between the gas pores and the ionomer phase at the membrane boundary, N_{H2O} (SI unit: mol/(m^2·s)), is defined using reaction source/sink terms in the catalytic layers:

$$\nabla_{\mathrm{H2O}} = k_{\mathrm{abs}}(a_{\mathrm{H2O,\,gas}} - a_{\mathrm{H2O,\,ionomer}}) \tag{5}$$

where k_{abs} (SI unit: mol/(m^2·s)) is an absorption rate constant.

In the gas phase, the water activity is defined as

$$a_{\mathrm{H2O,\,gas}} = \frac{x_{\mathrm{H2O,gas}}p}{p_{\mathrm{vapor}}} \tag{6}$$

where x_{H2O} (1) is the water molar fraction in the gas phase, p_{vapor} (SI unit: Pa) is the water vapor pressure, and p (SI unit: Pa) is the pressure.

Results and Discussion

Figure 4 shows the polarization plots (cell potential versus cell current density) for different relative humidities of the gases at the external GDL boundaries. Having both gas streams humidified to 95% results in the highest currents. The figure also shows that humidifying the anode to 95% and the cathode to 50% renders better performance than humidifying the anode to 50% and the cathode to 95%. 50% relative humidity on both electrodes results in the worst performance.

The open-circuit voltage around 0.95 V is significantly lower than the reversible potential of the cell reaction (approximately 1.18 V at 60°C). This is due to the cathodic polarization for oxygen reduction needed at open circuit to balance the parasitic hydrogen oxidation reaction on the cathode side due to the hydrogen transport through the membrane.

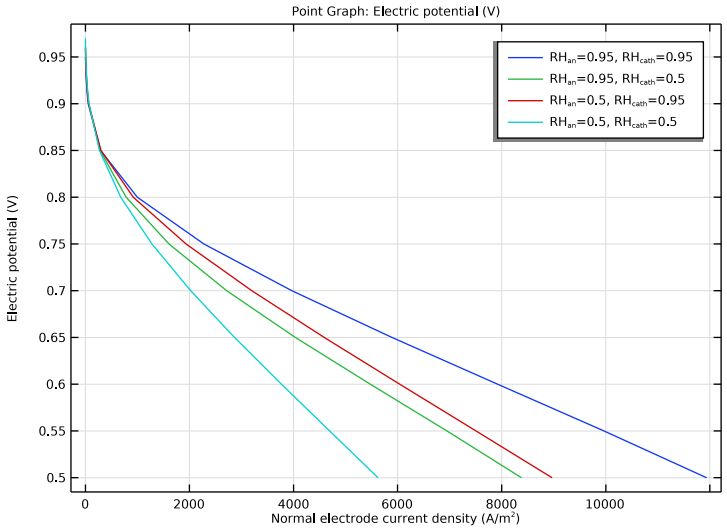


Figure 4: Polarization plots for various relative humidities of the gases in the anode and cathode compartments.

Figure 5 and Figure 6 show the water activity for the different humidity levels for the cell operating at 0.5 V and the corresponding ionomer conductivity, respectively. The anode humidified to 70% and the cathode to 95% results in a higher membrane conductivity than for the opposite 95%-70% anode-cathode case, thus explaining the differences in cell performance seen in Figure 4.

shows the temperature profile in the fuel cell. A temperature increase of about 3C is observed for the highest current level. This temperature increase explains the generally lower relative humidity levels seen in the central parts of the MEA compared to the outer parts of the GDLs seen in Figure 5.

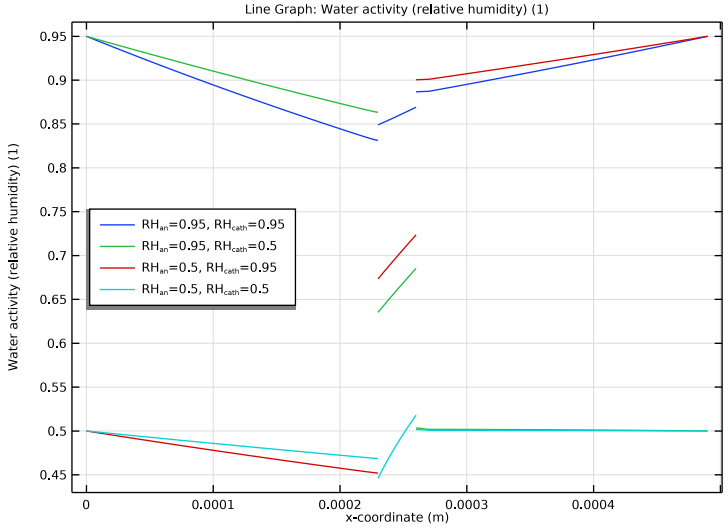


Figure 5: Water activity in the ionomer and gas phases for varied relative humidities and the cell operating at 0.5 V.

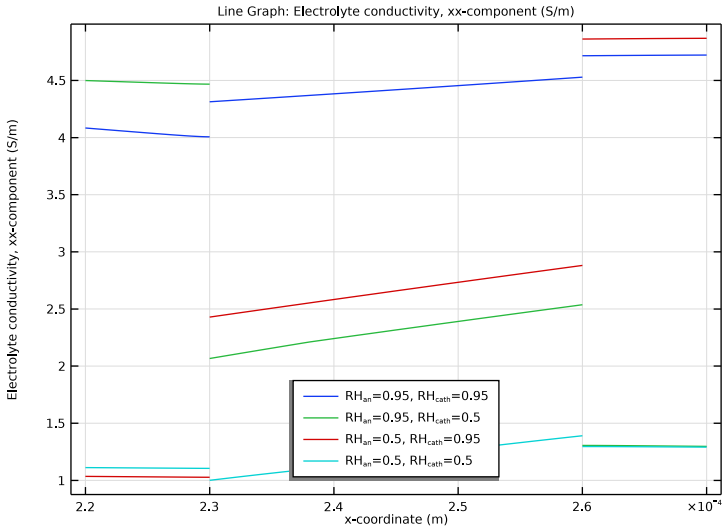


Figure 6: Ionomer conductivity for varied relative humidities and the cell operating at 0.5 V.

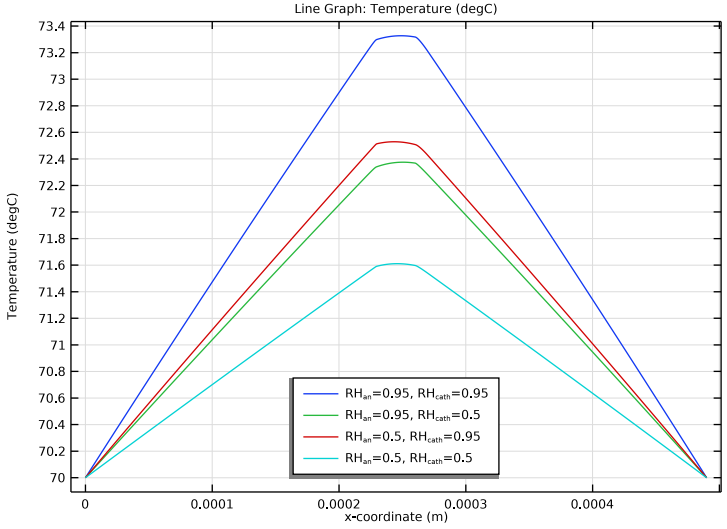


Figure 7: Temperature profile in the MEA for the cell operating at 0.5 V.

Application Library path: `Fuel_Cell_and_Electrolyzer_Module/Fuel_Cells/pem_mea_1d`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **1D**.

2 In the **Select Physics** tree, select **Electrochemistry>Hydrogen Fuel Cells>Proton Exchange (fc)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Heat Transfer>Heat Transfer in Solids (ht)**.

5 Click **Add**.

6 Click **Study**.

7 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Hydrogen Fuel Cell>Stationary with Initialization**.

8 Click **Done**.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `pem_mea_1d_parameters.txt`.

GEOMETRY 1

Construct the model geometry using seven separate intervals.

Anode GDL

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Anode GDL` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
0
L_GDL

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Anode MPL

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Anode MPL` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
L_GDL
L_GDL+L_MPL

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Anode CL

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Anode CL` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
L_GDL+L_MPL
L_GDL+L_MPL+L_CL

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Membrane

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Membrane` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
L_GDL+L_MPL+L_CL
L_GDL+L_MPL+L_CL+L_mem

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Cathode CL

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Cathode CL` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
L_GDL+L_MPL+L_CL+L_mem
L_GDL+L_MPL+L_CL+L_mem+L_CL

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Cathode MPL

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Cathode MPL` in the **Label** text field.

3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
L_GDL+L_MPL+L_CL+L_mem+L_CL
L_GDL+L_MPL+L_CL+L_mem+L_CL+L_MPL

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

Cathode GDL

1 Right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, type `Cathode GDL` in the **Label** text field.

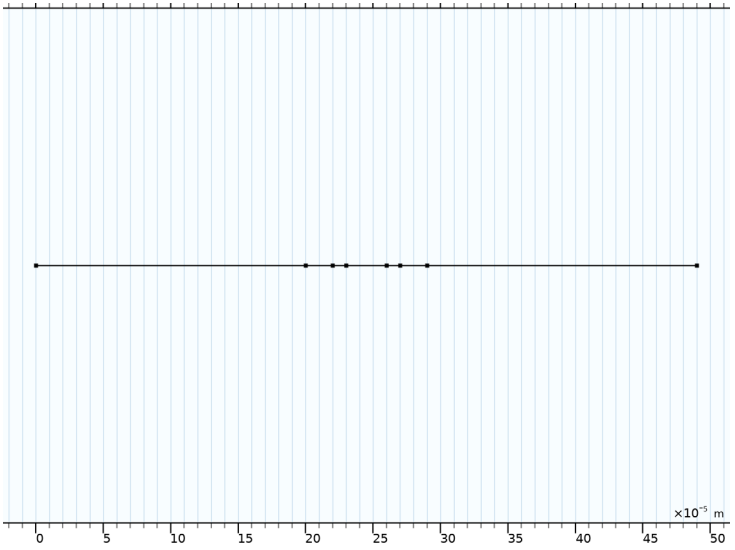
3 Locate the **Interval** section. In the table, enter the following settings:

Coordinates (m)
L_GDL+L_MPL+L_CL+L_mem+L_CL+L_MPL
L_GDL+L_MPL+L_CL+L_mem+L_CL+L_MPL+L_GDL

4 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

5 Click **Build All Objects**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.



DEFINITIONS

Now create some union selections, using the selections that were created in the geometry node by enabling the Resulting objects selection check box.

Anode Gas Compartment

1 In the **Definitions** toolbar, click **Union**.

2 In the **Settings** window for **Union**, type `Anode Gas Compartment` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Anode GDL**, **Anode MPL**, and **Anode CL**.

5 Click **OK**.

Cathode Gas Compartment

1 In the **Definitions** toolbar, click  **Union**.

2 In the **Settings** window for **Union**, type `Cathode Gas Compartment` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click + **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Cathode CL**, **Cathode MPL**, and **Cathode GDL**.

5 Click **OK**.

Ionomer Domains

1 In the **Definitions** toolbar, click  **Union**.

2 In the **Settings** window for **Union**, type `Ionomer Domains` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click + **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Anode CL**, **Membrane**, and **Cathode CL**.

5 Click **OK**.

CLs

1 In the **Definitions** toolbar, click  **Union**.

2 In the **Settings** window for **Union**, type `CLs` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click + **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Anode CL** and **Cathode CL**.

5 Click **OK**.

MPLs

1 In the **Definitions** toolbar, click  **Union**.

2 In the **Settings** window for **Union**, type `MPLs` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click + **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Anode MPL** and **Cathode MPL**.

5 Click **OK**.

GDLs

1 In the **Definitions** toolbar, click  **Union**.

2 In the **Settings** window for **Union**, type `GDLs` in the **Label** text field.

3 Locate the **Input Entities** section. Under **Selections to add**, click + **Add**.

4 In the **Add** dialog box, in the **Selections to add** list, choose **Anode GDL** and **Cathode GDL**.

5 Click **OK**.

MATERIALS

This model uses a polymer electrolyte material (Nafion) which is available in the material library. Add the material twice, and assign it first to the ionomer domains, and next to the membrane boundaries adjacent to the gas phase nodes. The boundary instance of the material will be used to provide rate constants for the water absorption-desorption reactions.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Fuel Cell and Electrolyzer>Polymer Electrolytes>Nafion, EW 1100, Vapor Equilibrated, Protonated**.

4 Right-click and choose **Add to Component 1 (comp1)**.

MATERIALS

Nafion, EW 1100, Vapor Equilibrated, Protonated (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Nafion, EW 1100, Vapor Equilibrated, Protonated (mat1)**.

2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

3 From the **Selection** list, choose **Ionomer Domains**.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Fuel Cell and Electrolyzer>Polymer Electrolytes>Nafion, EW 1100, Vapor Equilibrated, Protonated**.

3 Right-click and choose **Add to Component 1 (comp1)**.

4 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Nafion, EW 1100, Vapor Equilibrated, Protonated 1 (mat2)

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Geometric entity level** list, choose **Boundary**.

3 Select Boundaries 4 and 5 only.

HYDROGEN FUEL CELL (FC)

Set up the current distribution and transport model. Include mass transport using Maxwell-Stefan diffusion and momentum transport using Darcy's Law in both the anode and cathode gas mixtures. Additionally, include crossover of hydrogen and oxygen and electroosmotic water drag in the membrane. Note that the default gas species are hydrogen and water on the anode side, and oxygen, nitrogen and water on the cathode side. Start with adding the relevant domain nodes.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Hydrogen Fuel Cell (fc)**.

2 In the **Settings** window for **Hydrogen Fuel Cell**, locate the **H2 Gas Mixture** section.

3 Find the **Transport mechanisms** subsection. Select the **Use Darcy's Law for momentum transport** check box.

4 Locate the **O2 Gas Mixture** section. Select the **Use Darcy's Law for momentum transport** check box.

5 Click to expand the **Membrane Transport** section. Select the **H2** check box.

6 Select the **O2** check box.

7 Select the **Electroosmotic water drag** check box.

Membrane 1

1 In the **Physics** toolbar, click — **Domains** and choose **Membrane**.

2 In the **Settings** window for **Membrane**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Membrane**.

H2 Gas Diffusion Electrode 1

1 In the **Physics** toolbar, click — **Domains** and choose **H2 Gas Diffusion Electrode**.

2 In the **Settings** window for **H2 Gas Diffusion Electrode**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Anode CL**.

H2 Gas Diffusion Layer 1

1 In the **Physics** toolbar, click — **Domains** and choose **H2 Gas Diffusion Layer**.

2 In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Anode MPL**.

H2 Gas Diffusion Layer 2

1 In the **Physics** toolbar, click — **Domains** and choose **H2 Gas Diffusion Layer**.

2 In the **Settings** window for **H2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Anode GDL**.

O2 Gas Diffusion Electrode 1

1 In the **Physics** toolbar, click — **Domains** and choose **O2 Gas Diffusion Electrode**.

2 In the **Settings** window for **O2 Gas Diffusion Electrode**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Cathode CL**.

O2 Gas Diffusion Layer 1

1 In the **Physics** toolbar, click — **Domains** and choose **O2 Gas Diffusion Layer**.

2 In the **Settings** window for **O2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Cathode MPL**.

O2 Gas Diffusion Layer 2

1 In the **Physics** toolbar, click — **Domains** and choose **O2 Gas Diffusion Layer**.

2 In the **Settings** window for **O2 Gas Diffusion Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Cathode GDL**.

In the **Electrolyte Phase** node, the electrolyte conductivity is set to be taken from the **Materials** node. Inspect the settings in the **H2 Gas Phase** and **O2 Gas Phase** nodes. Note that the density and viscosity of the gas mixture, and the binary diffusion coefficients are calculated automatically when the respective default settings are used.

The properties for hydrogen and oxygen crossover and electroosmotic water drag in the **Membrane** node and in the child nodes that added by default are automatically taken from the **Materials** node.

Initial Values 1

1 In the **Model Builder** window, expand the **Membrane 1** node, then click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T_0 text field, type `T0`.

H2 Gas Diffusion Electrode 1

Set up the properties of the **H2 Gas Diffusion Electrode** node. The details of electrode kinetics are set in the child node. Note that the reference equilibrium potential is calculated automatically when the default **Built in** option is used.

1 In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **H2 Gas Diffusion Electrode 1**.

2 In the **Settings** window for **H2 Gas Diffusion Electrode**, locate the **Electrode Charge Transport** section.

3 In the σ_s text field, type `sigmas_CL`.

4 Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type `epsl_CL`.

5 Locate the **Gas Transport** section. In the ε_g text field, type `epsg_CL`.

6 In the κ_g text field, type `kappag_CL`.

H2 Gas Diffusion Electrode Reaction 1

1 In the **Model Builder** window, click **H2 Gas Diffusion Electrode Reaction 1**.

2 In the **Settings** window for **H2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.

3 In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_H2`.

4 Locate the **Active Specific Surface Area** section. In the a_v text field, type `a_CL`.

H2 Gas Diffusion Layer 1 - MPL

Set up the properties of the anode microporous layer and the anode gas diffusion layer in the **H2 Gas Diffusion Layer** nodes.

1 In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **H2 Gas Diffusion Layer 1**.

2 In the **Settings** window for **H2 Gas Diffusion Layer**, type `H2 Gas Diffusion Layer 1 - MPL` in the **Label** text field.

3 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_MPL`.

4 Locate the **Gas Transport** section. In the ε_g text field, type `epsg_MPL`.

5 In the κ_g text field, type `kappag_MPL`.

H2 Gas Diffusion Layer 2 - GDL

1 In the **Model Builder** window, click **H2 Gas Diffusion Layer 2**.

2 In the **Settings** window for **H2 Gas Diffusion Layer**, type `H2 Gas Diffusion Layer 2 - GDL` in the **Label** text field.

3 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_GDL`.

4 Locate the **Gas Transport** section. In the ε_g text field, type `epsg_GDL`.

5 In the κ_g text field, type `kappag_GDL`.

O2 Gas Diffusion Electrode 1

Set up the properties of the **O2 Gas Diffusion Electrode** node. The details of electrode kinetics are set in the child node. Note that the reference equilibrium potential is calculated automatically when the default **Built in** option is used.

1. In the **Model Builder** window, click **O2 Gas Diffusion Electrode 1**.
2. In the **Settings** window for **O2 Gas Diffusion Electrode**, locate the **Electrode Charge Transport** section.
3. In the σ_s text field, type `sigmas_CL`.
4. Locate the **Effective Electrolyte Charge Transport** section. In the ε_l text field, type `epsl_CL`.
5. Locate the **Gas Transport** section. In the ε_g text field, type `epsg_CL`.
6. In the κ_g text field, type `kappag_CL`.

O2 Gas Diffusion Electrode Reaction 1

1. In the **Model Builder** window, click **O2 Gas Diffusion Electrode Reaction 1**.
2. In the **Settings** window for **O2 Gas Diffusion Electrode Reaction**, locate the **Electrode Kinetics** section.
3. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0_O2`.
4. In the α_a text field, type `alphaa_O2`.
5. Locate the **Active Specific Surface Area** section. In the a_v text field, type `a_CL`.

O2 Gas Diffusion Layer 1 - MPL

Set up the properties of the cathode microporous layer and the cathode gas diffusion layer in the **O2 Gas Diffusion Layer** nodes.

1. In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)** click **O2 Gas Diffusion Layer 1**.
2. In the **Settings** window for **O2 Gas Diffusion Layer**, type `O2 Gas Diffusion Layer 1 - MPL` in the **Label** text field.
3. Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_MPL`.
4. Locate the **Gas Transport** section. In the ε_g text field, type `epsg_MPL`.
5. In the κ_g text field, type `kappag_MPL`.

O2 Gas Diffusion Layer 2 - GDL

1. In the **Model Builder** window, click **O2 Gas Diffusion Layer 2**.
2. In the **Settings** window for **O2 Gas Diffusion Layer**, type `O2 Gas Diffusion Layer 2 - GDL` in the **Label** text field.

3 Locate the **Electrode Charge Transport** section. In the σ_s text field, type `sigmas_GDL`.

4 Locate the **Gas Transport** section. In the ε_g text field, type `epsg_GDL`.

5 In the κ_g text field, type `kappag_GDL`.

Finally, set up the boundary conditions and initial values.

Electronic Conducting Phase 1

In the **Model Builder** window, click **Electronic Conducting Phase 1**.

Electric Ground 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Ground**.

2 Select Boundary 1 only.

Electronic Conducting Phase 1

In the **Model Builder** window, click **Electronic Conducting Phase 1**.

Electric Potential 1

1 In the **Physics** toolbar, click **Attributes** and choose **Electric Potential**.

2 Select Boundary 8 only.

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the $\phi_{s,bnd}$ text field, type `E_cell`.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)> H2 Gas Phase 1** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Composition** section.

3 From the **Mixture specification** list, choose **Humidified mixture**.

4 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH_an`.

5 In the T_{hum} text field, type `T0`.

H2 Gas Phase 1

In the **Model Builder** window, click **H2 Gas Phase 1**.

H2 Inlet 1

1 In the **Physics** toolbar, click **Attributes** and choose **H2 Inlet**.

2 Select Boundary 1 only.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Hydrogen Fuel Cell (fc)> O2 Gas Phase 1** click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Composition** section.

3 From the **Mixture specification** list, choose **Humidified air**.

4 In the $\mathrm{RH}_{\mathrm{hum}}$ text field, type `RH_cath`.

5 In the T_{hum} text field, type `T0`.

O2 Gas Phase 1

In the **Model Builder** window, click **O2 Gas Phase 1**.

O2 Inlet 1

1 In the **Physics** toolbar, click **Attributes** and choose **O2 Inlet**.

2 Select Boundary 8 only.

Now set up the Heat Transfer physics. The Nafion material contains data for the thermal conductivity in the membrane. Use user-defined thermal conductivities for the other domains.

HEAT TRANSFER IN SOLIDS (HT)

In the **Model Builder** window, under **Component 1 (comp1)** click **Heat Transfer in Solids (ht)**.

Solid 2 - GDLs

1 In the **Physics** toolbar, click **Domains** and choose **Solid**.

2 In the **Settings** window for **Solid**, type `Solid 2 - GDLs` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **GDLs**.

4 Locate the **Heat Conduction, Solid** section. From the k list, choose **User defined**. In the associated text field, type `kappa_GDL`.

Solid 3 - MPLs

1 In the **Physics** toolbar, click **Domains** and choose **Solid**.

2 In the **Settings** window for **Solid**, type `Solid 3 - MPLs` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **MPLs**.

4 Locate the **Heat Conduction, Solid** section. From the k list, choose **User defined**. In the associated text field, type `kappa_MPL`.

Solid 4 - CLs

1 In the **Physics** toolbar, click **Domains** and choose **Solid**.

2 In the **Settings** window for **Solid**, type `Solid 4 - CLs` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **CLs**.

4 Locate the **Heat Conduction, Solid** section. From the *k* list, choose **User defined**. In the associated text field, type `kappa_CL`.

The Solid 1 node that was added by default should now be active on the membrane domain only.

Solid 1 - Membrane

1 In the **Model Builder** window, click **Solid 1**.

2 In the **Settings** window for **Solid**, type `Solid 1 - Membrane` in the **Label** text field.

Note that the Nafion material node under Materials is marked with a red cross, indicating an undefined material property. The missing material properties are the density and heat capacity, which are however not needed for the stationary study we will be making.

Make the density and heat capacity user defined in all domains order to remove the red cross.

3 Locate the **Thermodynamics, Solid** section. From the ρ list, choose **User defined**. From the C_p list, choose **User defined**.

Solid 2 - GDLs

1 In the **Model Builder** window, click **Solid 2 - GDLs**.

2 In the **Settings** window for **Solid**, locate the **Thermodynamics, Solid** section.

3 From the ρ list, choose **User defined**. From the C_p list, choose **User defined**.

Solid 3 - MPLs

1 In the **Model Builder** window, click **Solid 3 - MPLs**.

2 In the **Settings** window for **Solid**, locate the **Thermodynamics, Solid** section.

3 From the ρ list, choose **User defined**. From the C_p list, choose **User defined**.

Solid 4 - CLs

1 In the **Model Builder** window, click **Solid 4 - CLs**.

2 In the **Settings** window for **Solid**, locate the **Thermodynamics, Solid** section.

3 From the ρ list, choose **User defined**. From the C_p list, choose **User defined**.

Temperature 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

Finalize the heat transfer physics by setting the external temperature and the initial condition.

2 Select Boundaries 1 and 8 only.

3 In the **Settings** window for **Temperature**, locate the **Temperature** section.

4 In the T_0 text field, type `T0`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type `T0`.

MULTIPHYSICS

Electrochemical Heating 1 (ech1)

In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain> Electrochemical Heating**.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extra fine**.

4 Locate the **Sequence Type** section. From the list, choose **User-controlled mesh**.

Distribution 1

1 In the **Model Builder** window, right-click **Edge 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **CLs**.

4 Locate the **Distribution** section. In the **Number of elements** text field, type `10`.

5 Click  **Build All**.

STUDY 1

Parametric Sweep

1 In the **Study** toolbar, click  **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click  **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
RH_an (Inlet relative humidity, anode)	`0.95 0.5`	1

5 Click + **Add**.

6 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
RH_cath (Inlet relative humidity, cathode)	`0.95 0.5`	1

7 From the **Sweep type** list, choose **All combinations**.

Step 2: Stationary

1 In the **Model Builder** window, click **Step 2: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click + **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
E_cell (Cell potential)	`range(1.0,-0.01,0.91)` `range(0.9,-0.05,0.5)`	V

6 In the **Study** toolbar, click = **Compute**.

RESULTS

Polarization Plots

1 In the **Home** toolbar, click  **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Polarization Plots` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

Point Graph 1

1 Right-click **Polarization Plots** and choose **Point Graph**.

2 Select Boundary 8 only.

3 In the **Settings** window for **Point Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Hydrogen Fuel Cell>fc.phis - Electric potential - V**.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 Click **Replace Expression** in the upper-right corner of the **x-Axis Data** section. From the menu, choose **Component 1 (comp1)>Hydrogen Fuel Cell>fc.nls - Normal electrode current density - A/m²**.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

7 Find the **Include** subsection. Clear the **Point** check box.

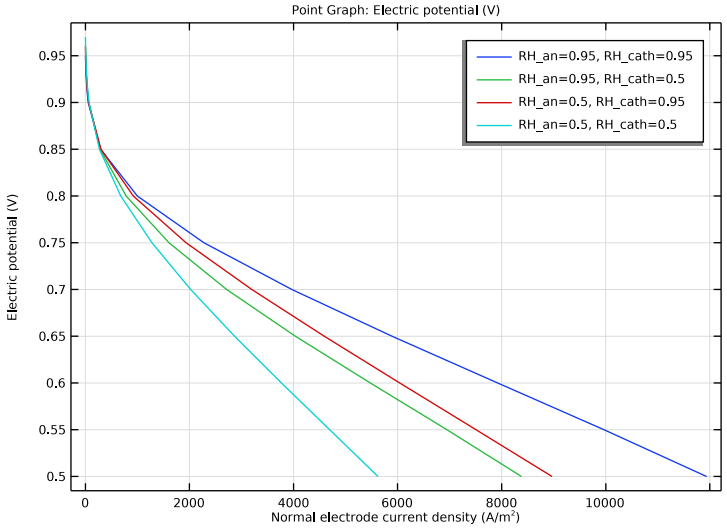
Filter 1

1 Right-click **Point Graph 1** and choose **Filter**.

2 In the **Settings** window for **Filter**, locate the **Point Selection** section.

3 In the **Logical expression for inclusion** text field, type `fc.nIs>0`.

4 In the **Polarization Plots** toolbar, click **Plot**.



Water Activity (Relative Humidity) (fc)

1 In the **Model Builder** window, under **Results** click **Water Activity (Relative Humidity) (fc)**.

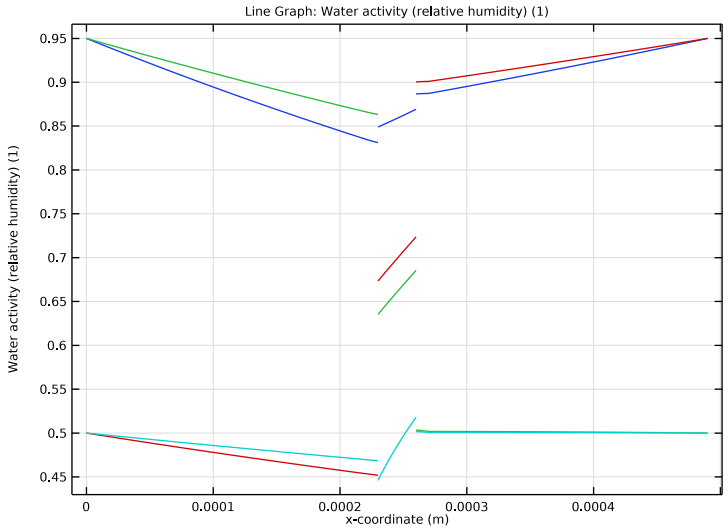
2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Parameter selection (E_cell)** list, choose **Last**.

Line Graph 1

1 In the **Model Builder** window, expand the **Water Activity (Relative Humidity) (fc)** node, then click **Line Graph 1**.

2 In the **Water Activity (Relative Humidity) (fc)** toolbar, click **Plot**.



Ionomer Conductivity

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Ionomer Conductivity` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol3)**.

4 From the **Parameter selection (E_cell)** list, choose **Last**.

Line Graph 1

1 Right-click **Ionomer Conductivity** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Hydrogen Fuel Cell>Electrolyte conductivity - S/m> fc.sigmaIxx - Electrolyte conductivity, xx-component**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Click to expand the **Legends** section. Select the **Show legends** check box.

8 In the **Ionomer Conductivity** toolbar, click **Plot**.